

Supporting Information Available

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5	UV spectrum of Phelligrider A (1)
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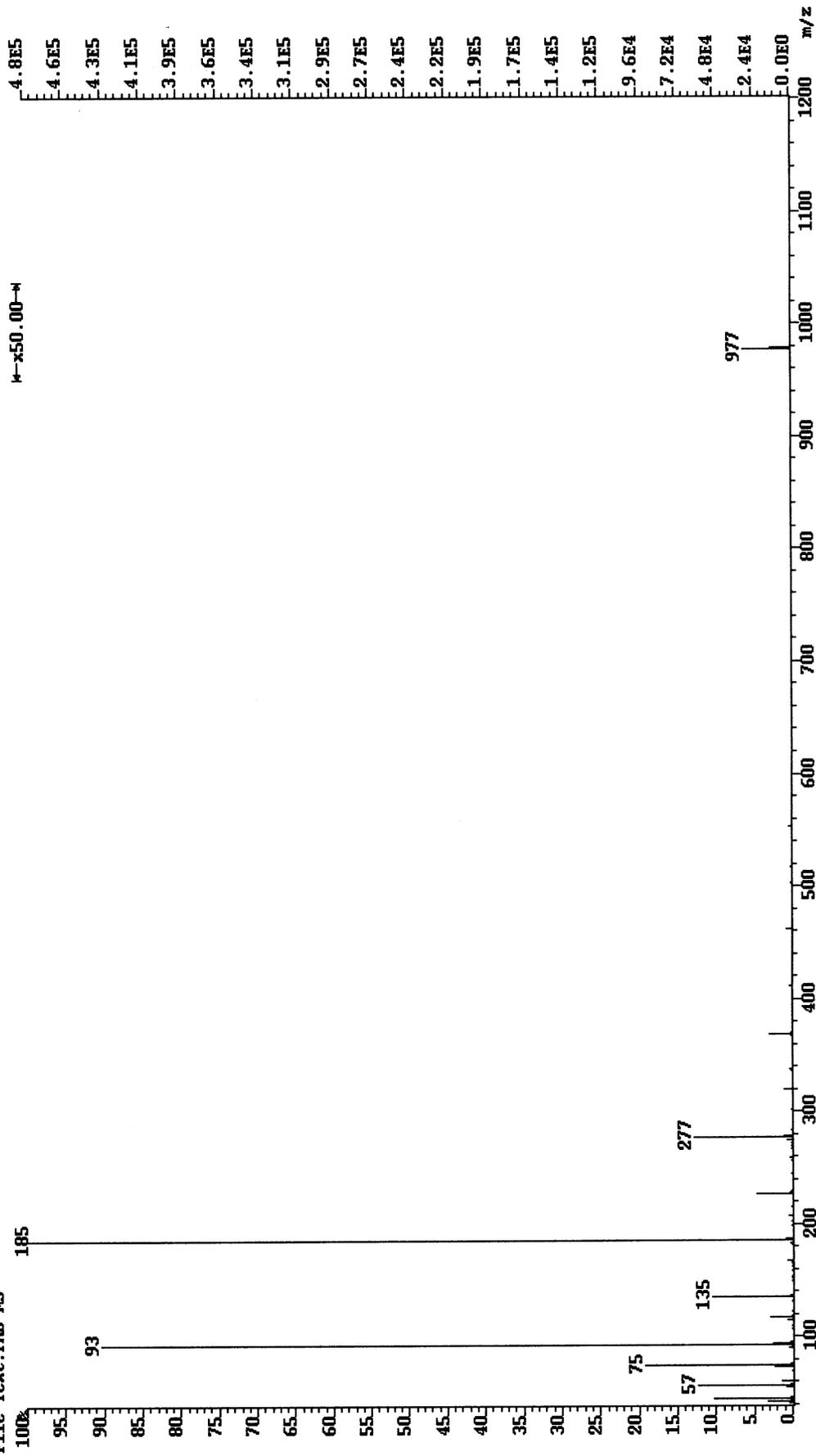
Manuscript Title: **Phelligrider A, A Highly Oxygenated and Unsaturated Twenty-Six Membered Macrocyclic Metabolite with Antioxidant Activity from the Fungus *Phellinus igniarius***

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File: WY-501 Ident: 2_14 Win 100PPM Acq: 30-NOV-2004 22:26:46 +0:48 Cal: FAB041202
Autospec-UltimaTOF FAB+ Magnet BpM: 185 BpI: 482225 TIC: 1418377 Flags: HALL
File Text: FAB-MS



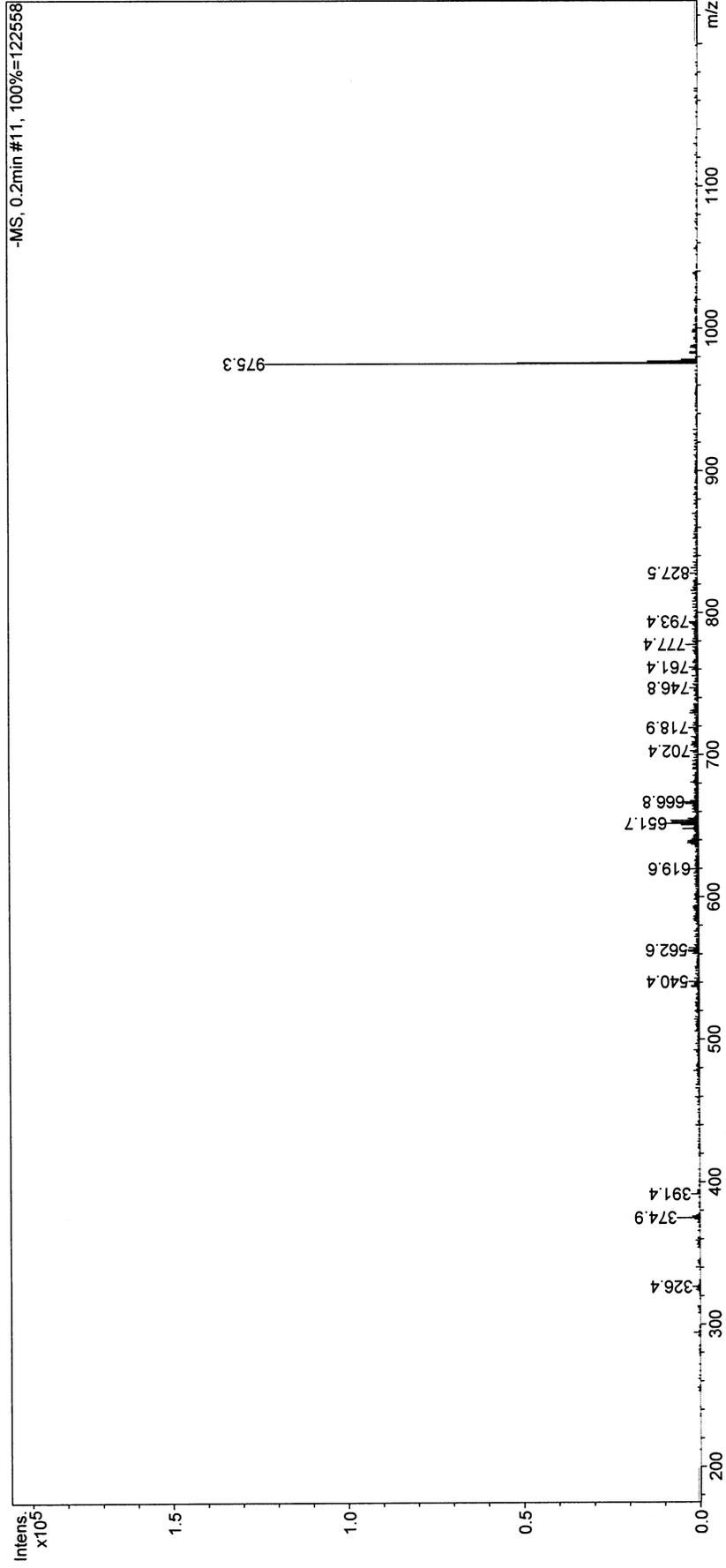
FAB-MS of compound 1

Display Report - Selected Window Selected Analysis

Analysis Name: wy-501.d
Method: TEST.MS
Sample Name: wy-501
Analysis Info:

Instrument: LC-MSD-Trap-SL
Operator: Administrator

Print Date: 11/16/2004 04:34:52 PM
Acq. Date: 11/12/2004 05:05:08 PM



Shanghai Institute of Organic Chemistry
Chinese Academic of Sciences
High Resolution MS Data Report



Instrument:



Bruker Daltonics, Inc.
APEXIII 7.0 TESLA FTMS

Card Serial Number: B041344

Sample Serial Number: WY-501

Operator: Liao Yuanxi Date: 2004/11/18

XMASS Mass Analysis for /Bruker/data/200411/B041344/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 977.1567440

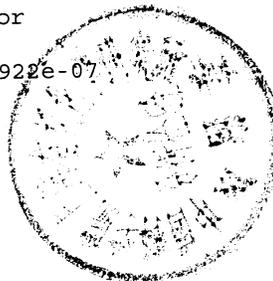
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DBE max = 36

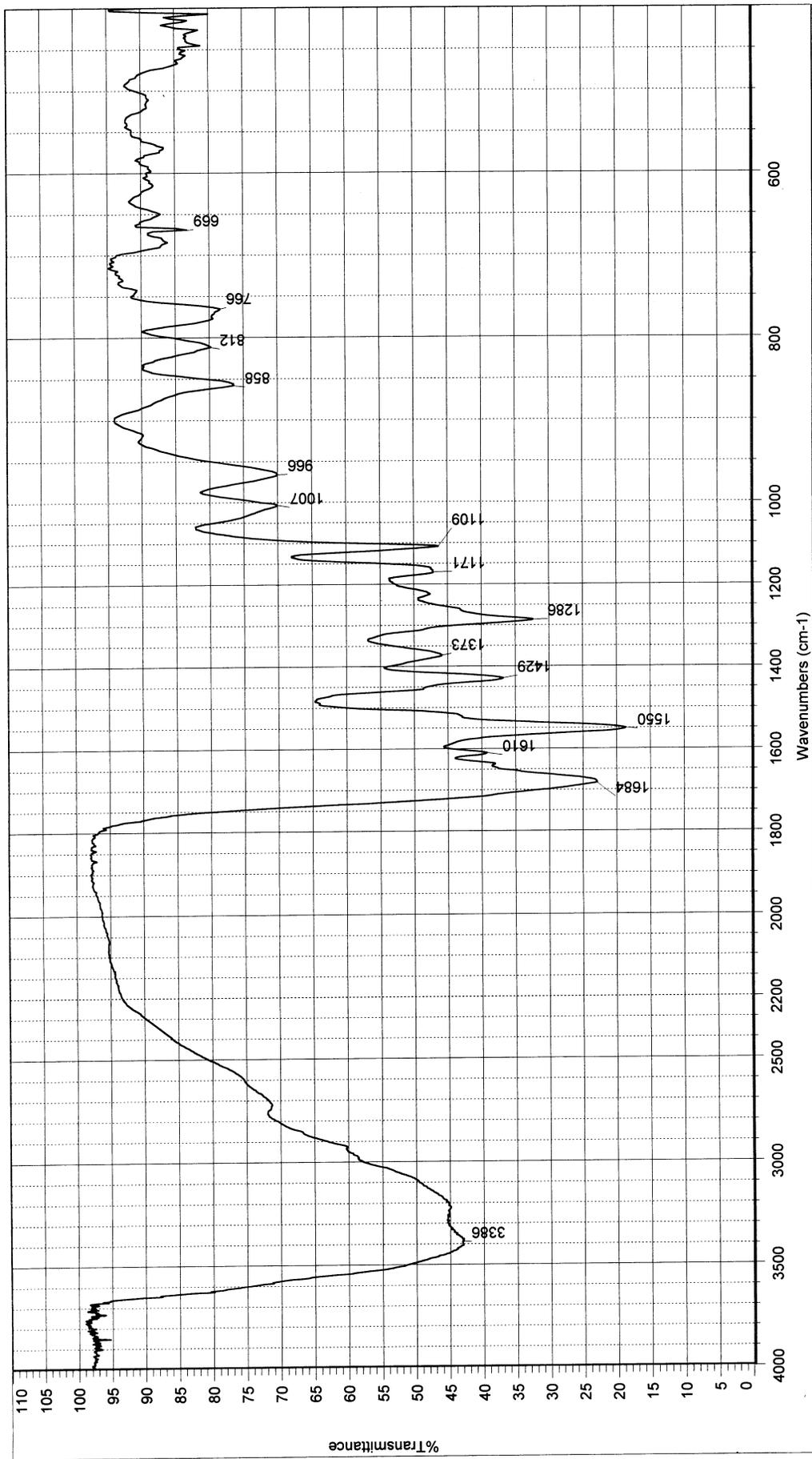
Max Candidates = 100

Atom	#(min, max)		Wt%(min, max)	
C	0	100	0.00	100.00
H	0	100	0.00	100.00
O	0	30	0.00	100.00

#	C	H	O	mass	DBE	error
***	Mass Analysis for mass 977.1567440					
1	52	33	20	977.1559699	36.5	7.922e-07



HR-MS of compound 1



Date: Thu Apr 01 11:06:37 2004

Sample Name: L10D (KBr)

Scans: 64

检测单位: 国家药物及代谢产物分析研究中心

Resolution: 4.000

检测仪器: 美国尼高力公司傅立叶变换红外光谱仪: IMPACT - 400

IR spectrum of compound 1

THERMO SPECTRONIC ~ VISION32 SOFTWARE V1.25

Batch Information - scan014

Batch Type Scan Operator Name (None Entered)
Instrument ID 110514 Aborted No

Results Table - scan014

Data Mode Absorbance

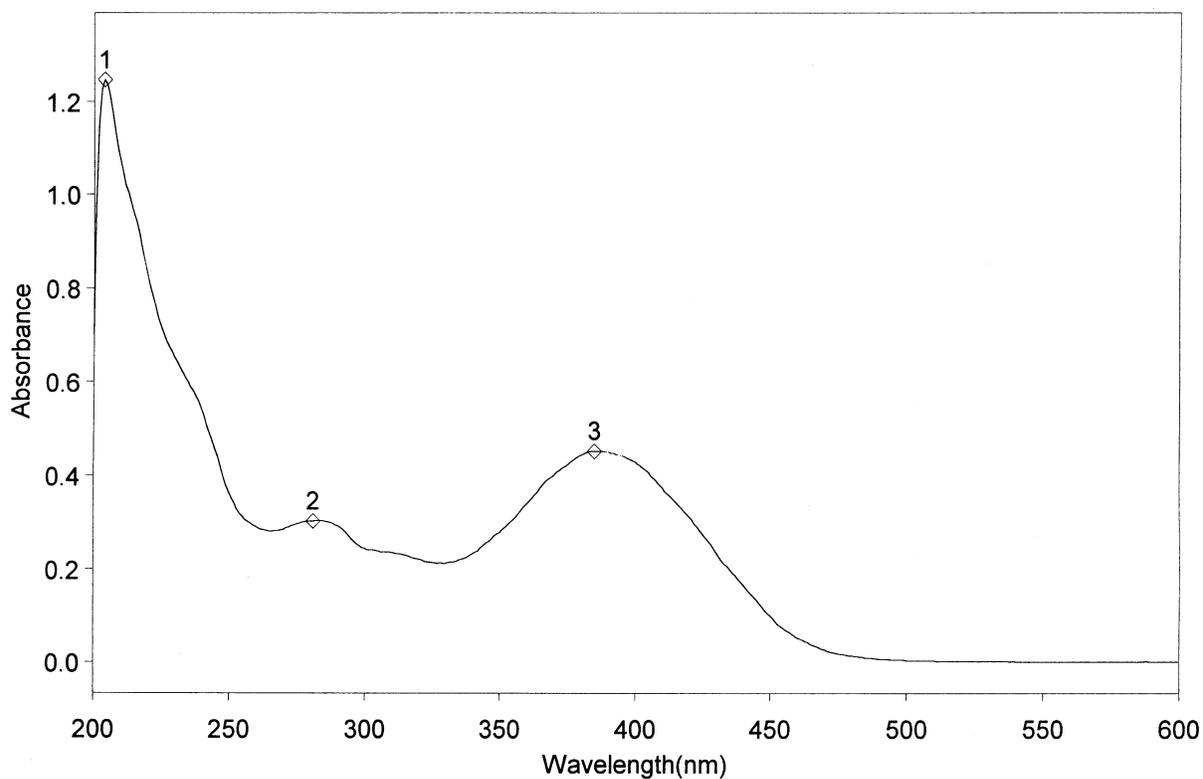
	A	B	C	D	E
1	L10D		1	2	3
2	Cycle01	nm	204.0	281.0	385.0
3	Manual	A	1.246	.302	.451

All calculations have been performed to double precision as defined by ANSI/IEEE STD 754-1985 but have been rounded for display purposes.

L10D

Description 0.114mg/10mlMeOH

L10D,Cycle01



UV spectrum of compound 1

INOVA-501 1H-NMR WY-11 IN DMSO 04.10.12

File: PROTON

9.497
9.180
9.127
9.091

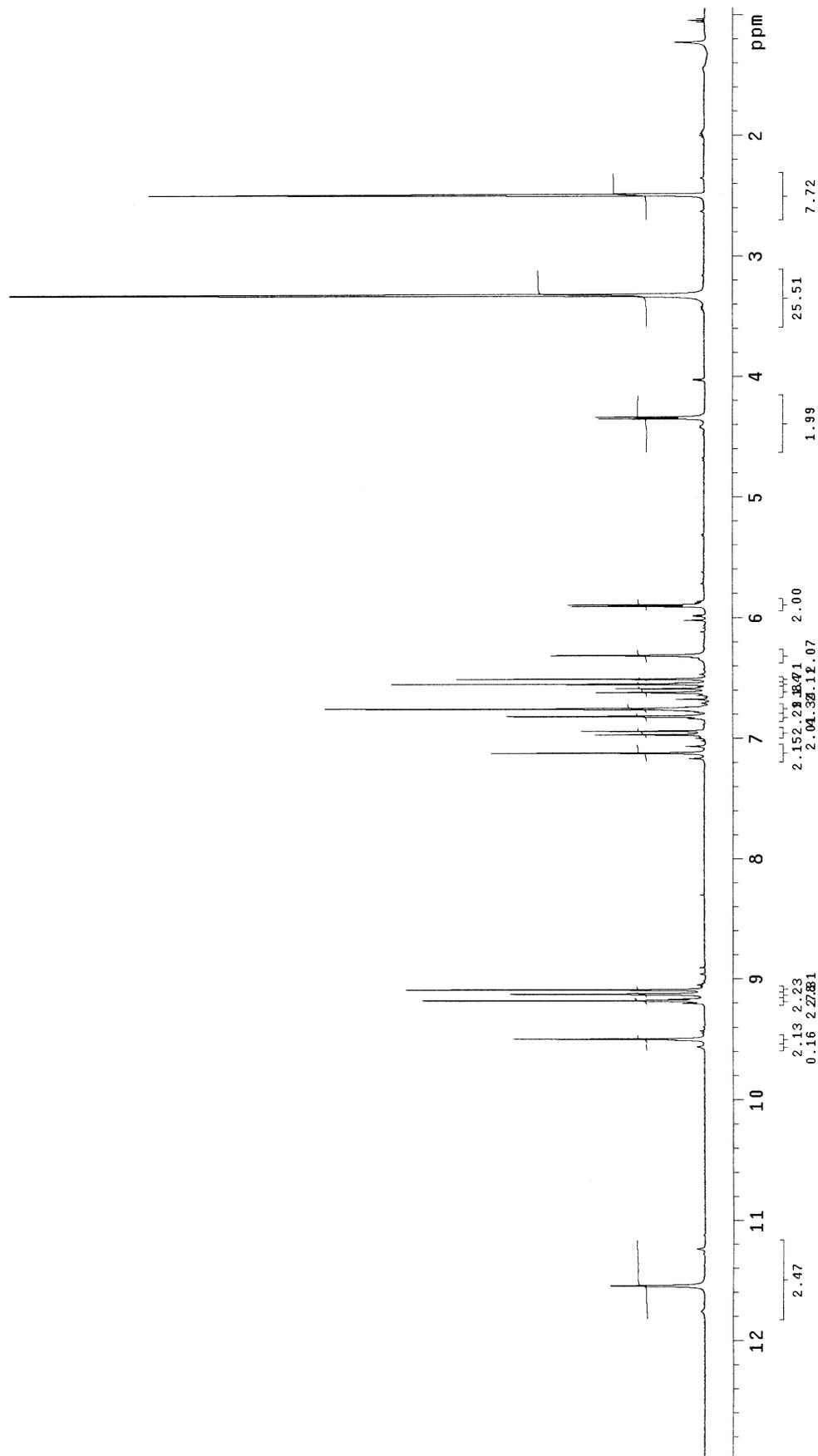
7.121
6.970
6.939
6.817
6.756
6.619
6.588
6.551
6.509
6.313
5.905
5.892

4.348
4.335

3.321
3.318

2.493
2.490
2.486

11.546



¹H NMR spectrum of compound 1

INOVA-501 1H-NMR WY-11 IN DMSO 04.10.12

File: PROTON

9.180
9.127
9.091

9.497

7.121

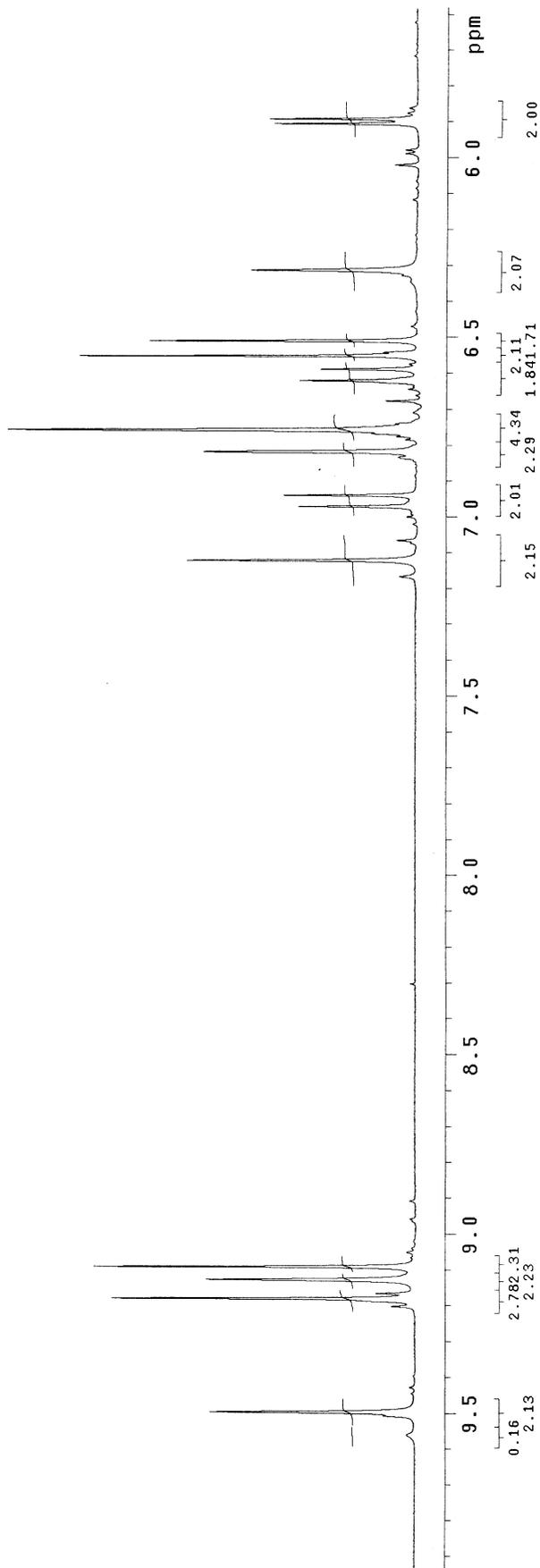
6.970
6.939

6.817
6.756

6.619
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6.509

6.313

5.905
5.892

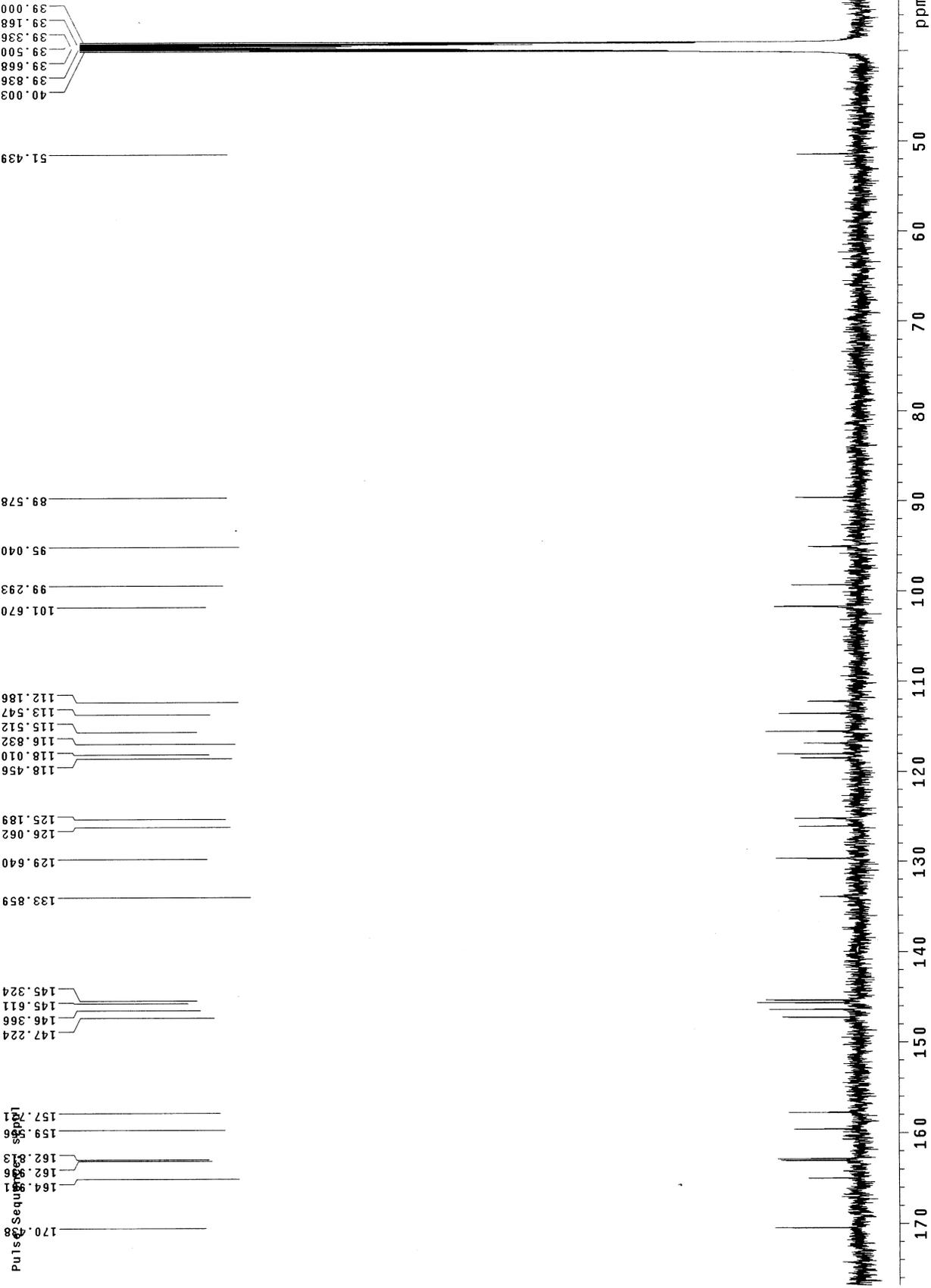


Regional enlarged 1H NMR spectrum of compound 1

INOVA-500 13C-NMR L10D1 IN DMSO

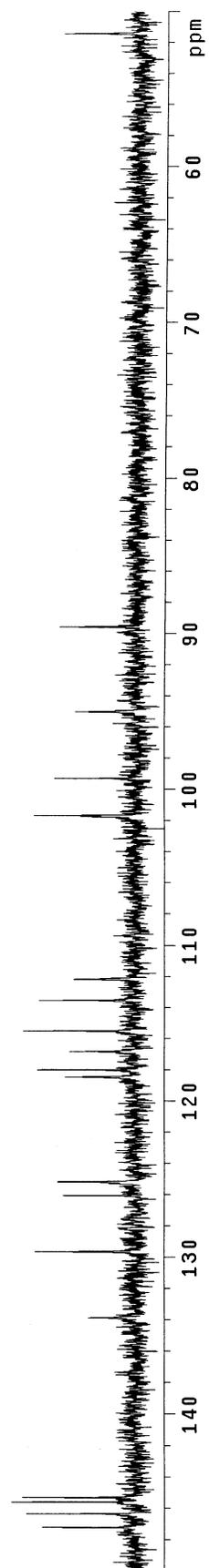
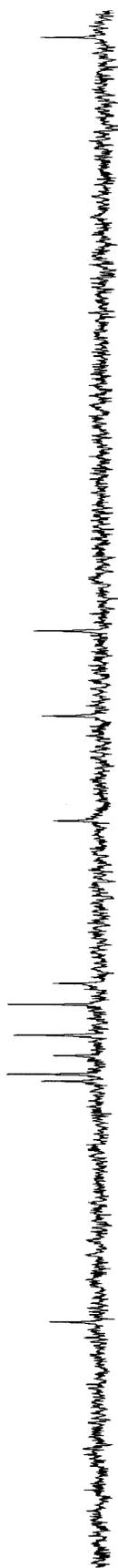
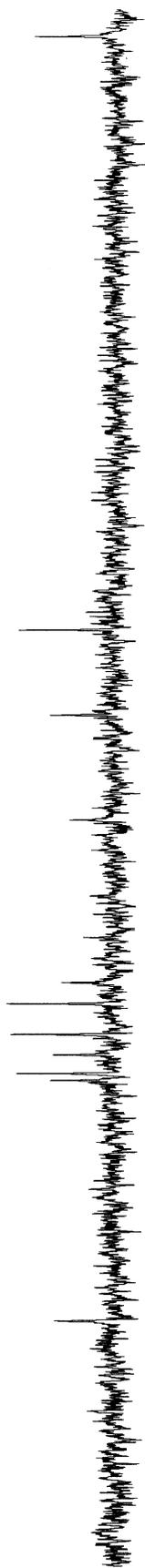
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Sample directory: auto_03Nov2004-15:15:15

Pulse Sequence: zgpg30



¹³C NMR spectrum of compound 1

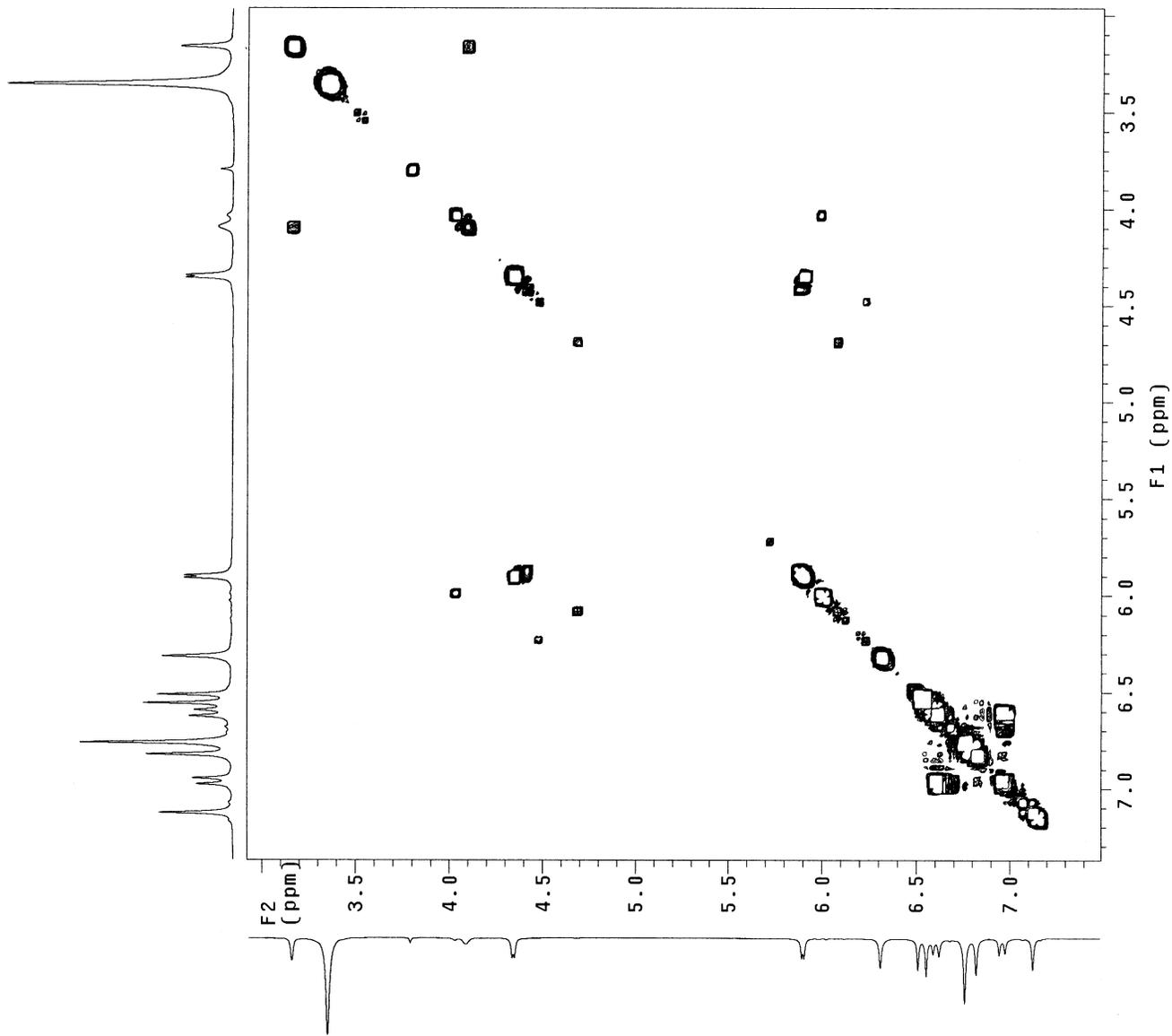
INOVA-500 DEPT-NMR L1001 IN DMSO
Archive directory: /export/home/autogc/vnmrSYS/data
Sample directory: auto_03Nov2004-15:15:15
Pulse Sequence: DEPT



DEPT spectrum of compound 1

INOVA-501 gCOSY L1001 IN DMSO 04.01.06

Solvent: DMSO
Temp: 25.0 C / 298.1 K
INOVA-500 "NMRS501"
Relax. delay 1.000 sec
Acq. time 0.198 sec
Width 5182.7 Hz
2D Width 5182.7 Hz
4 repetitions
256 increments
OBSERVE H1 499.7474027 MHZ
DATA PROCESSING
Ss sine bell 0.099 sec
F1 DATA PROCESSING
Ss sine bell 0.025 sec
FT size 2048 x 2048
Total time 21 min, 24 sec

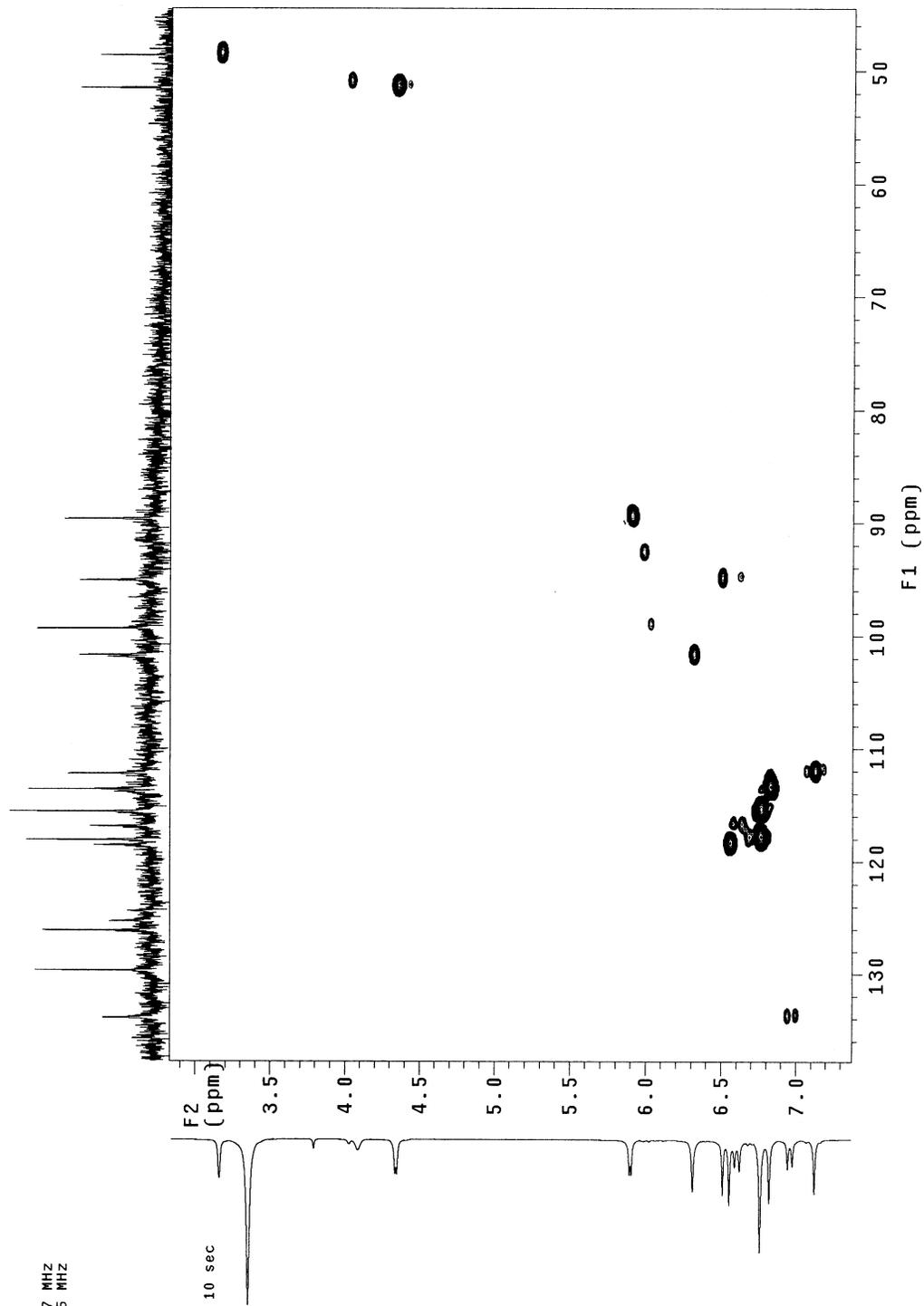


^1H - ^1H COSY spectrum of compound **1**

File: CARBON

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "NMRS01"

Relax. delay 1.000 sec
Acq. time 0.205 sec
Width 4985.0 Hz
2D Width 21367.5 Hz
64 repetitions
192 increments
OBSERVE H1, 499.7474027 MHz
DECUPLE C13, 125.6734815 MHz
Power 48 dB
on during acquisition
off during delay
GARP modulated
DATA PROCESSING
Sine bell 0.032 sec
F1 DATA PROCESSING
Sine bell 0.005 sec
F1 size 2048 x 4096
Total time 4 hr, 23 min, 10 sec

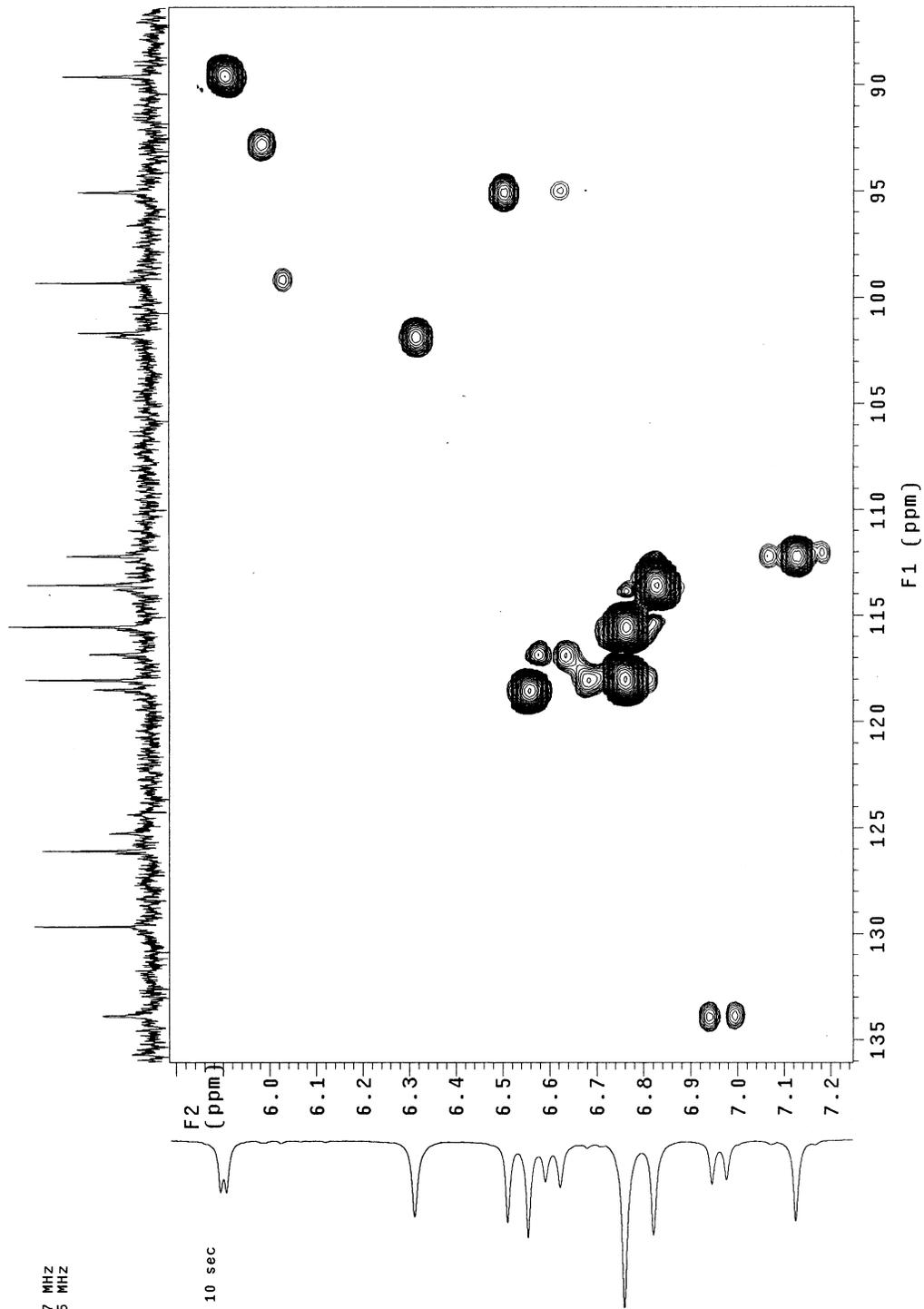


HSQC spectrum of compound 1

File: CARBON

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: I-14-87
INOVA-500 "MNR501"

Relax. delay 1.000 sec
Acq. time 0.205 sec
Width 4985.0 Hz
2D Width 21367.5 Hz
64 repetitions
192 increments
OBSERVE H1 499.7474027 MHZ
DECOUPLE C13, 125.6734815 MHZ
Power 48 dB,
on during acquisition
off during delay
GARP-1 modulated
DATA PROCESSING
Sine bell 0.032 sec
F2 DATA PROCESSING
Sine bell 0.005 sec
F1 size 2048 x 4096
Total time 4 hr, 23 min, 10 sec

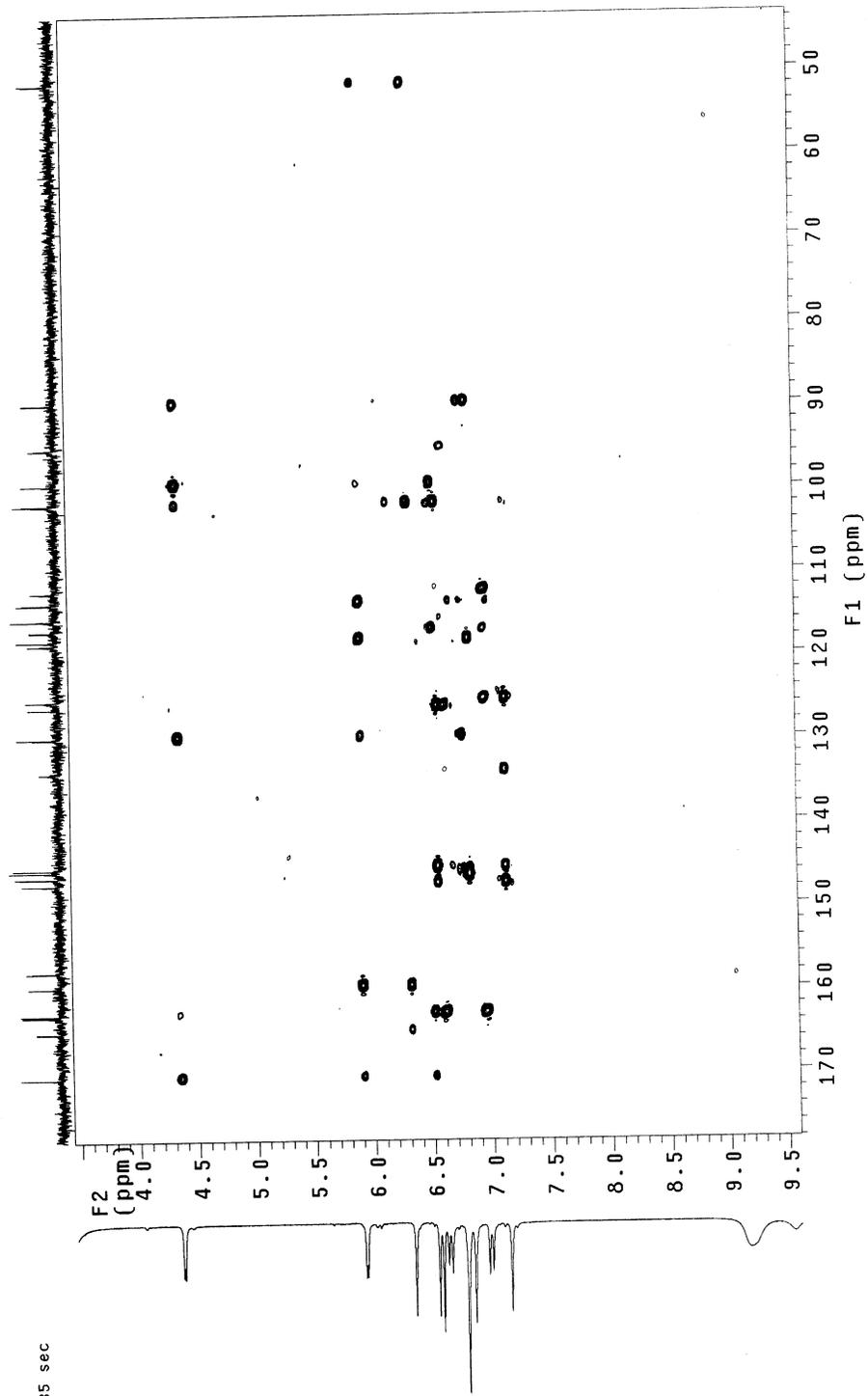


Regional enlarged HSQC spectrum of compound **1**

INOVA-501 gHMC L1001 IN DMSO 04.11.02

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: 1-14-87
File: HMC DMSO1102-L1001
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.186 sec
Width 5497.5 Hz
2D Width 19138.8 Hz
16 repetitions
320 increments
OBSERVE F1 499.7474033 MHZ
DATA PROCESSING
Sine bell 0.045 sec
F1 DATA PROCESSING
Sine bell 0.007 sec
F1 size 2048 x 4096
Total time 1 hr, 49 min, 35 sec

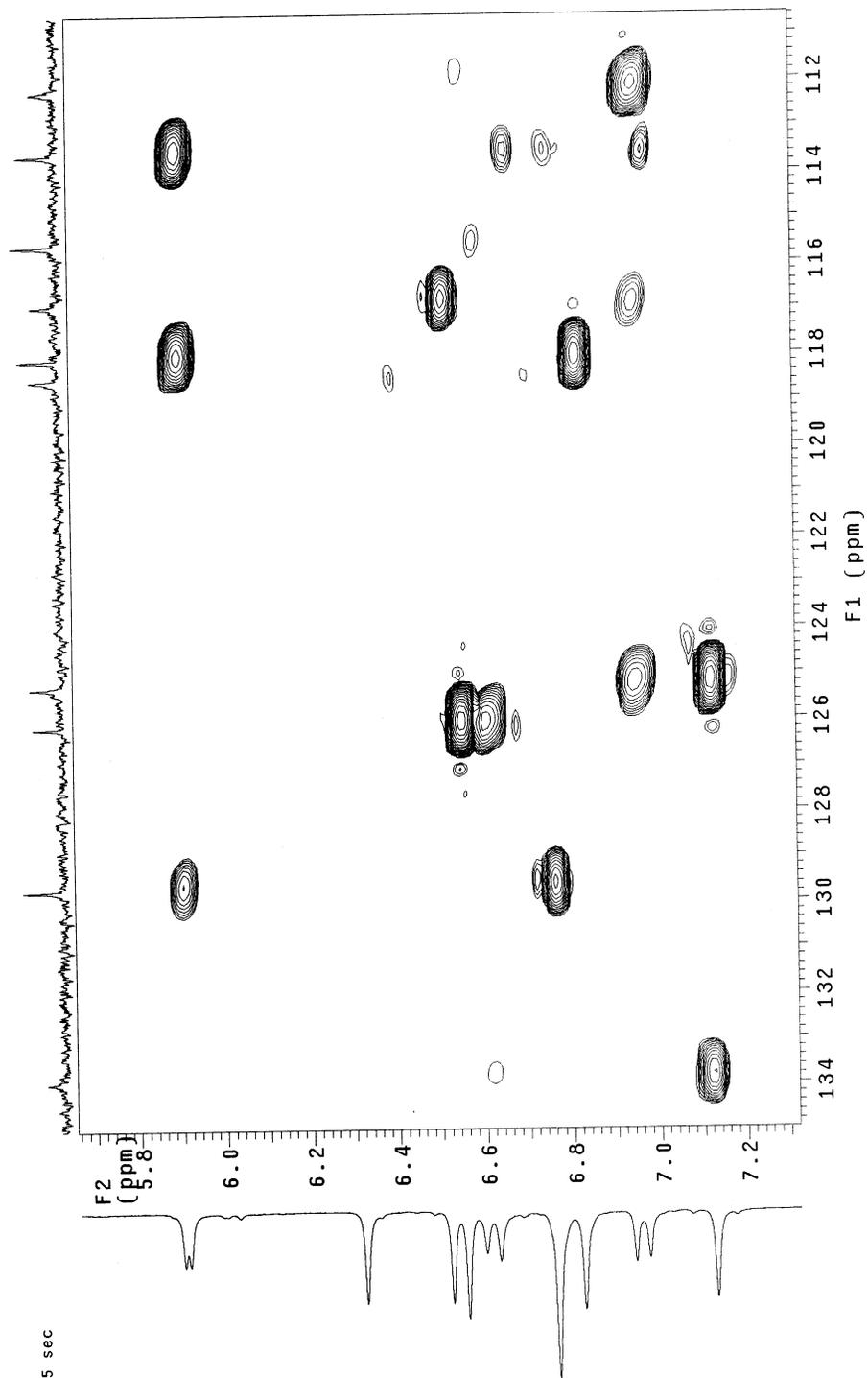


HMC spectrum of compound 1

INOVA-501 gHMBC L1001 IN DMSO 04.11.02

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: i-14-87-1102-L1001
File: HBCDMSO1102-L1001
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.186 sec
Width 5497.5 Hz
2D Width 19138.8 Hz
16 repetitions
320 increments
OBSERVE H1, 499.7474033 MHz
DATA PROCESSING
Sine bell 0.045 sec
F1 DATA PROCESSING
Sine bell 0.007 sec
F1 size 2048 X 4096
Total time 1 hr, 49 min, 35 sec

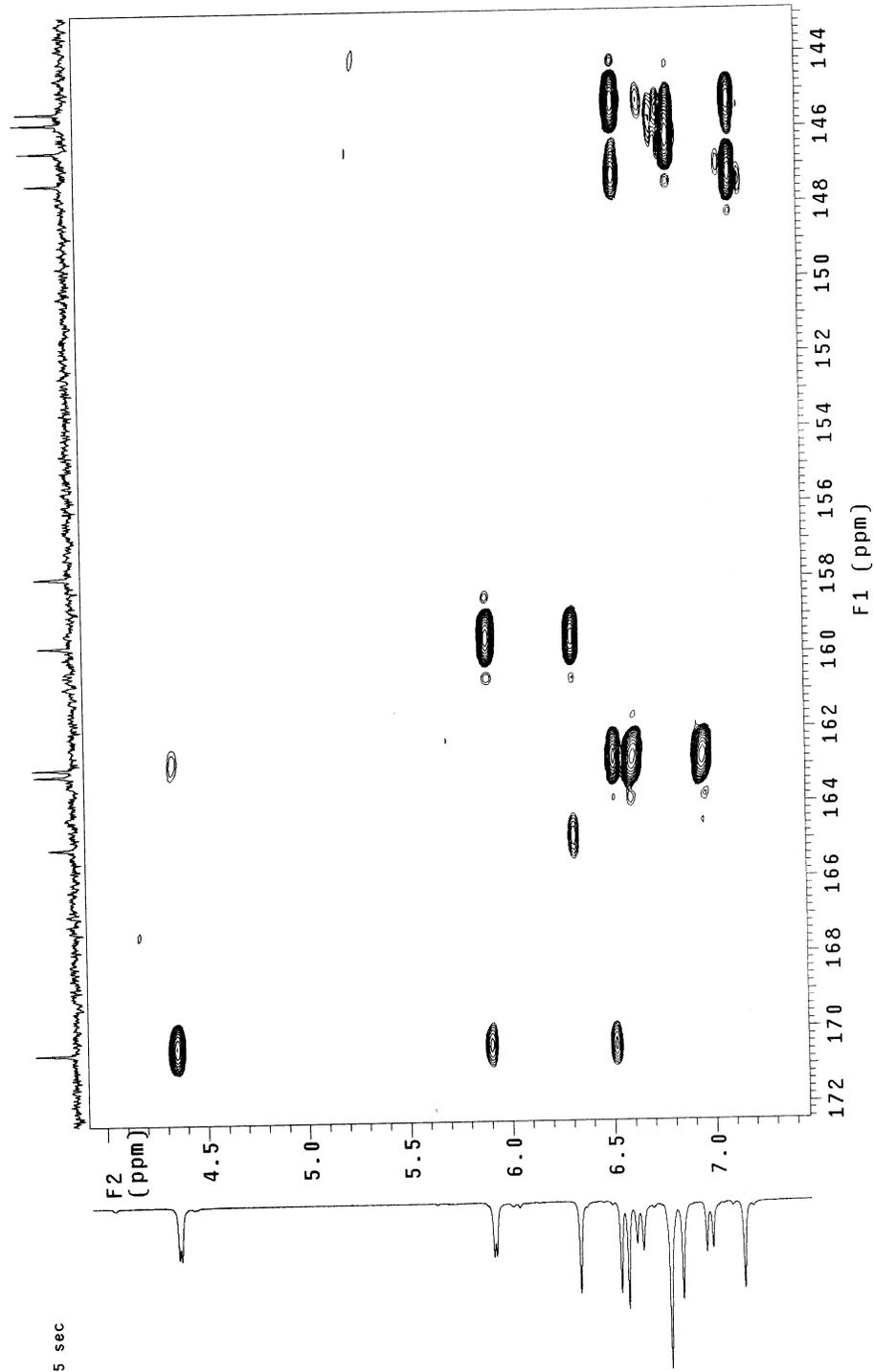


Regional enlarged HMBC spectrum of compound 1

INOVA-501 gHMBC L1001 IN DMSO 04.11.02

Solvent: DMSO
Temp. 25.0 C / 288.1 K
User: j-4487
File: HMBCDMSO1102-L1001
INOVA-500 "NHR501"

Relax. delay 1.000 sec
Acq. time 0.186 sec
Width 5497.5 Hz
2D Width 19138.8 Hz
16 repetitions
320 increments
OBSERVE H1, 499.7474033 MHZ
DATA PROCESSING
Sine bell 0.045 sec
F1 DATA PROCESSING
Sine bell 0.007 sec
F1 size 2048 X 4096
Total time 1 hr, 49 min, 35 sec

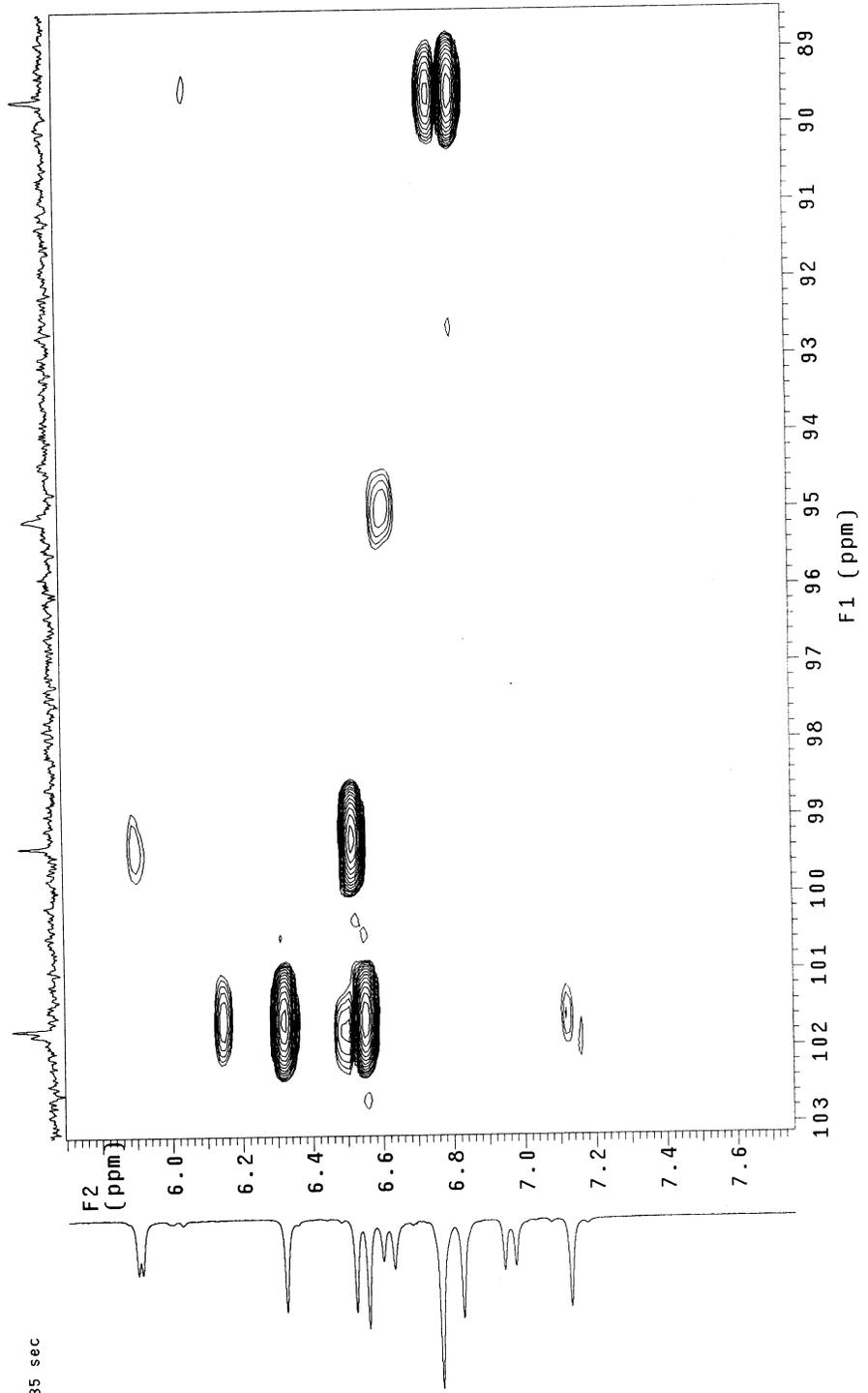


Regional enlarged HMBC spectrum of compound 1

INOVA-501 gHMBC L1001 IN DMSO 04.11.02

Solvent: DMSO
Temp. 25.0 C / 298.1 K
User: j-44-871102-L1001
File: HMBCDMSO1102-L1001
INOVA-500 "NHR501"

Relax. delay 1.000 sec
Acq. time 0.186 sec
Width 5497.5 Hz
2D Width 19138.8 Hz
16 repetitions
320 increments
OBSERVE H1, 499.7474033 MHZ
DATA PROCESSING
Sine bell 0.045 sec
F1 DATA PROCESSING
Sine bell 0.007 sec
F1 size 2048 X 4096
Total time 1 hr, 49 min, 35 sec



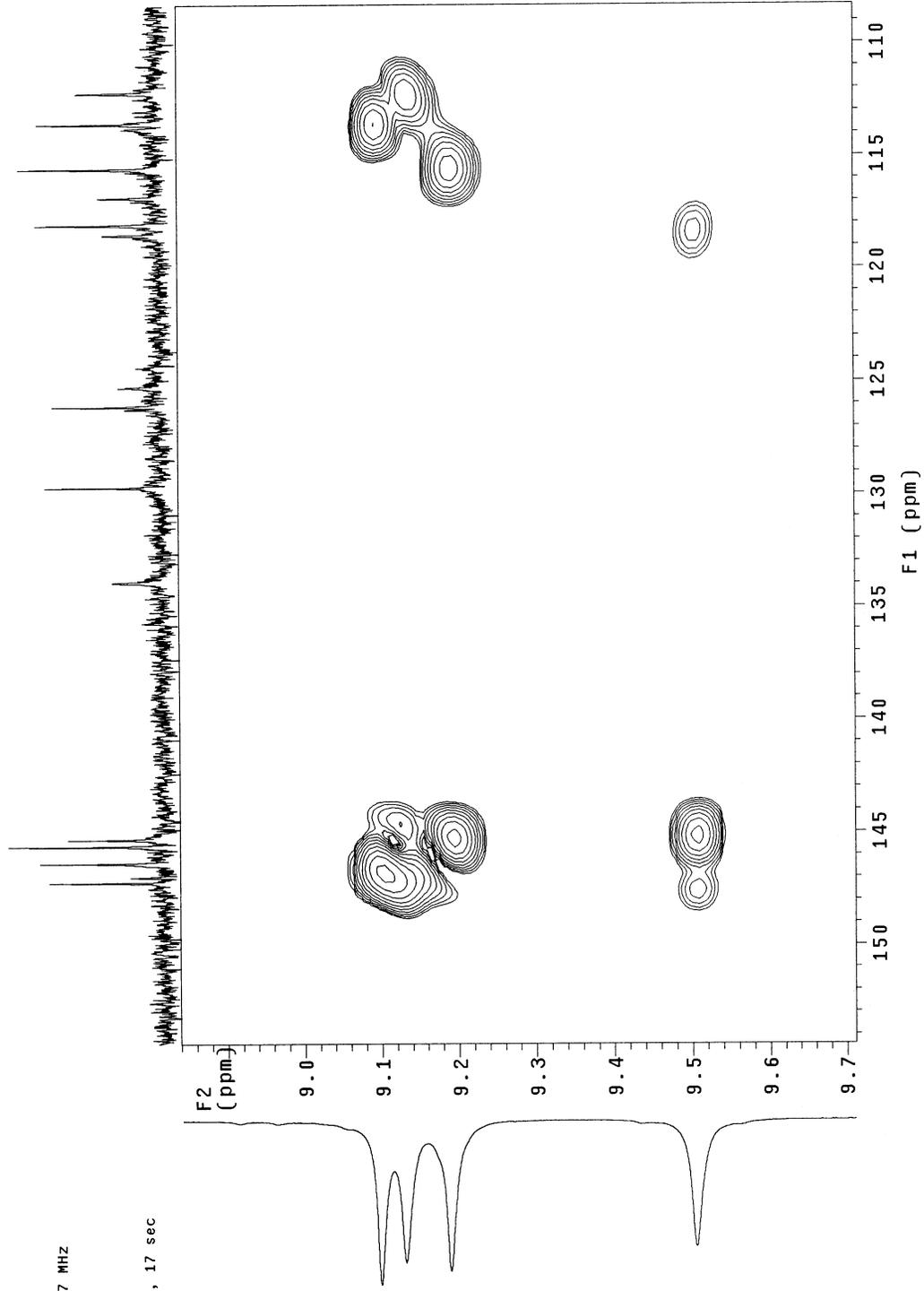
Regional enlarged HMBC spectrum of compound 1

INOVA-501_gHMBC_L10D1 IN DMSO 04.01.06

File: CARBON

Solvent: DMSO
Temp: 25.0 C / 298.1 K
User: 1-14-87
INOVA-500 "NMR501"

Relax. delay 1.000 sec
Acq. time 0.198 sec
Width 5182.7 Hz
2D Width 23923.4 Hz
128 repetitions
256 increments
OBSERVE H1, 499.7474027 MHZ
DATA PROCESSING
Sine bell 0.039 sec
F1 DATA PROCESSING
Sine bell 0.003 sec
FT size 2048 x 4096
Total time 11 hr, 42 min, 17 sec

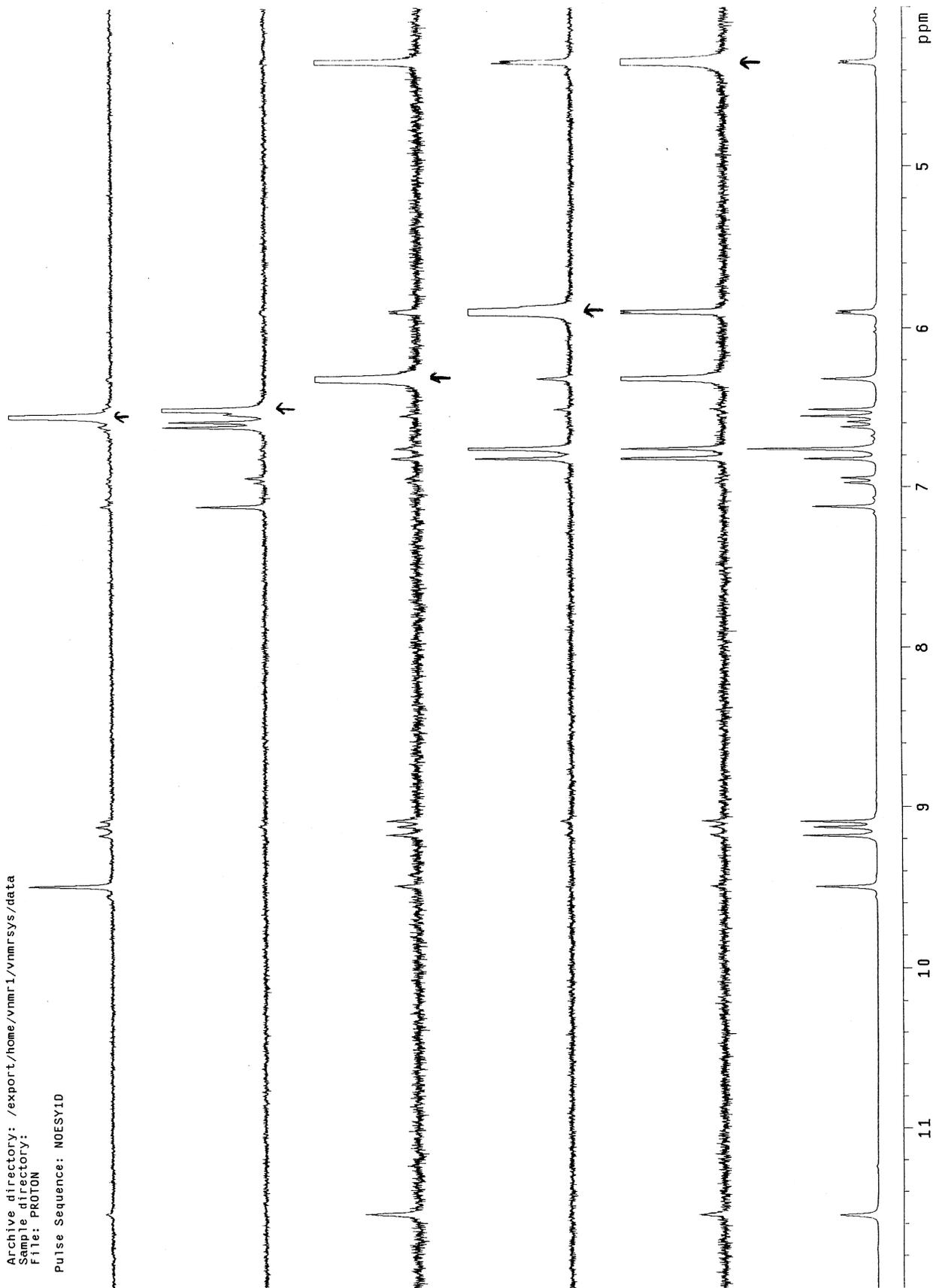


Regional enlarged HMBC spectrum of compound **1**

INOVA-500 NOESY1D-NMR WY-11 IN DMSO

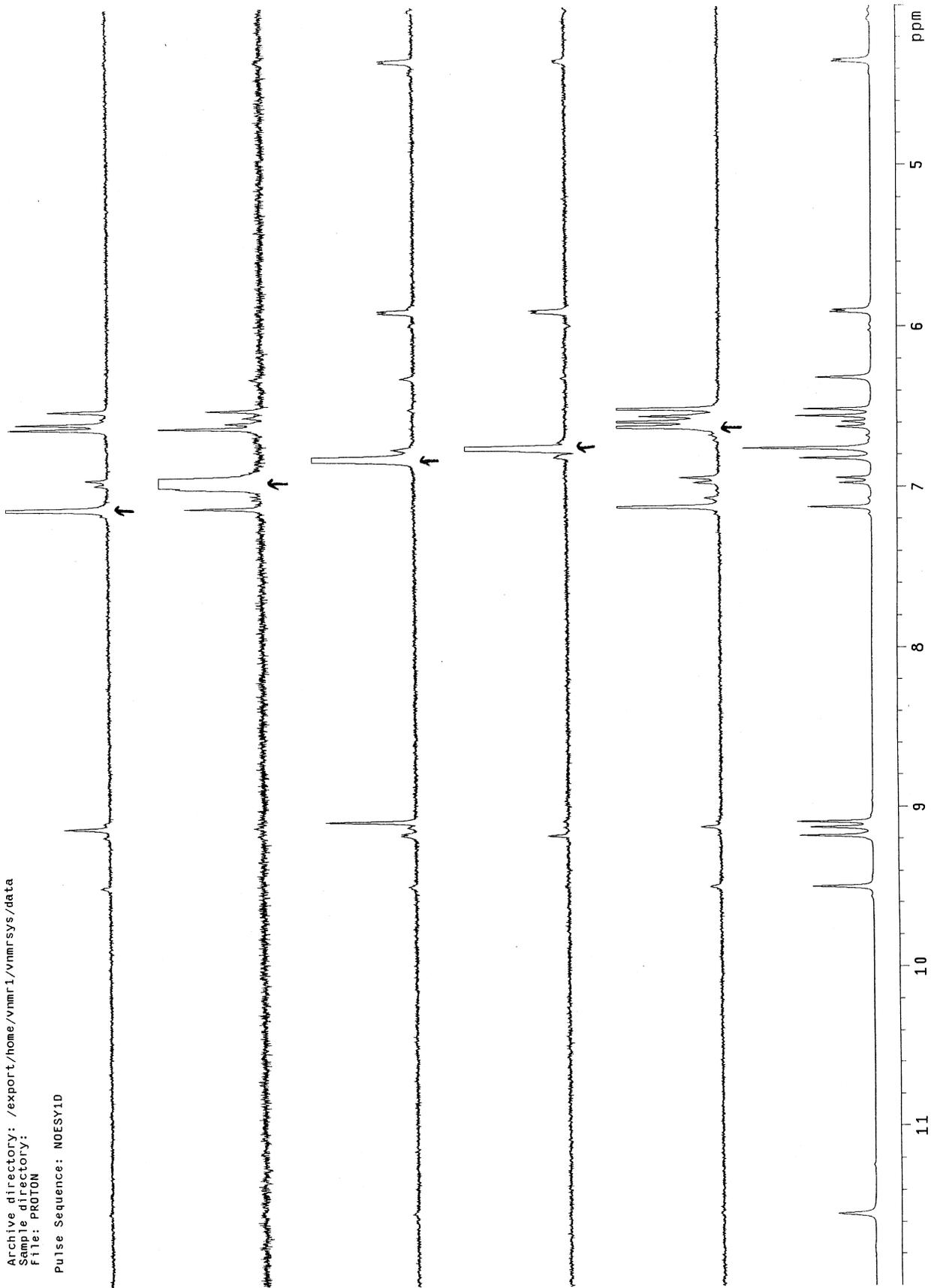
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Pulse Sequence: NOESY1D



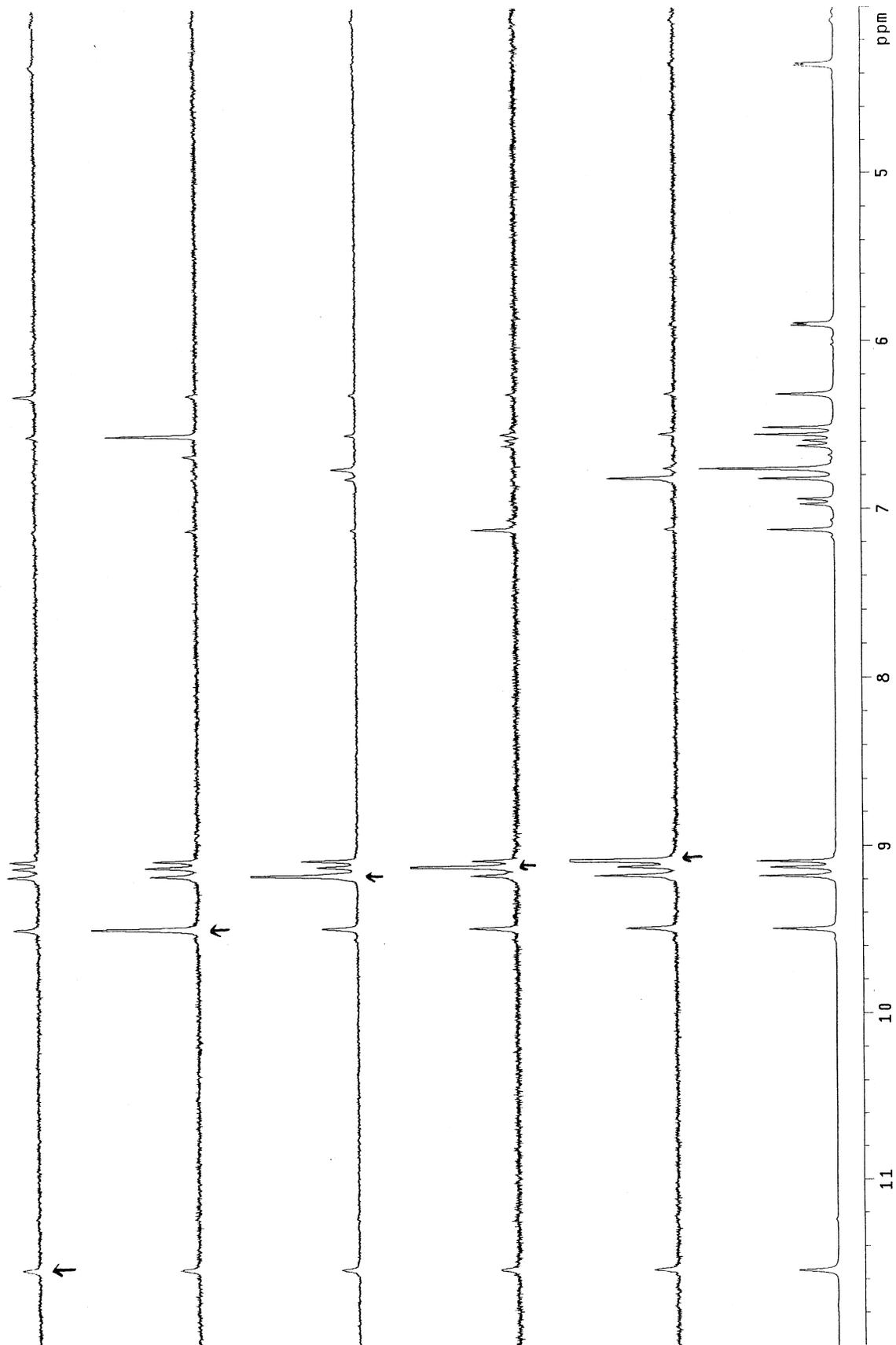
NOE difference spectrum 1 of compound 1

INOVA-500 NOESY1D-NMR WY-11 IN DMSO
Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory:
File: PROTON
Pulse Sequence: NOESY1D



NOE difference spectrum 2 of compound **1**

INOVA-500 NOESY1D-NMR WY-11 IN DMSO
Archive directory: /export/home/vnmr1/vnmrSYS/data
Sample directory:
File: PROTON
Pulse Sequence: NOESY1D



NOE difference spectrum 3 of compound 1

Table 1. ^1H and ^{13}C NMR data of compound **1**. (Recorded in DMSO- d_6)

No.	δ_{H}	δ_{C}	No.	δ_{H}	δ_{C}
2		163.0 s	2'		157.7 s
3		99.3 s	3'		101.7 s
4		170.4 s	4'		165.0 s
5	6.51 s	95.0 d	5'	6.31 s	101.7 d
6		162.8 s	6'		159.6 s
7	6.60 d 15.5	116.8 d	7'	4.34 d 6.5	51.4 d
8	6.95 d 15.5	133.9 d	8'	5.90 d 6.5	89.6 d
9		126.1 s	9'		129.6 s
10	7.12 s	112.2 d	10'	6.82 brs	113.5 d
11		145.3 s	11'		145.6 s
12		147.2 s	12'		146.4 s
13	6.55 s	118.5 d	13'	6.76 brs	115.5 d
14		125.2 s	14'	6.76 brs	118.0 d

NMR data were measured at 500 MHz for proton and at 125 MHz for carbon. The assignments were based on DEPT, ^1H - ^1H COSY, HSQC, HMBC and NOE difference experiments. $-\text{OH}$: δ 9.09 (brs, 11'- OH), 9.13 (brs, 11- OH), 9.18 (brs, 12'- OH), 9.50 (brs, 12- OH), 11.55 (brs, 4- OH).